CSCS

Annual Report
2018

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

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The photographer Alessandro Della Bella has portrayed eight staff members of CSCS: Nora Abi Akar, Stephanie Frequente, Miguel Gila, Katarzyna Pawlikowska, Angelo Mangili, Maxime Martinasso, Vasileios Karakasis, Rolando Summermatter.

Welcome from the Director

Thomas Schulthess, Director of CSCS.

As the new year starts, it is time to present the annual report of the previous year - and this means time to look back. What was important for me and my team? Instead of the usual greeting, I would like to share with you the questions I have been asked.

Are you glad 2018 is over?
Is it really over? It started in 2017 and will probably end in 2019.

Could you explain why?
The infrastructure work highlights of 2018 started in 2017, and detailed planning won't be completed before summer 2019. Important projects don't respect calendar boundaries.

What were your personal highlights at CSCS in 2018?
The list is long! Looking back from the future, it will probably be the decision of the ETH Board to keep CSCS' User Lab infrastructure on the roadmap of Swiss scientific research infrastructure based on strong recommendations conducted by the Swiss National Science Foundation; in practice, this means that the High-Performance Computing and Networking (HPCN) initiative that funds the supercomputing infrastructure at CSCS and extreme-scale application development in Switzerland will continue to receive financial support through 2024 at least. This gives us planning reliability, which is a huge advantage for the long-term development of the centre.

Were there also highlights in international High-Performance Computing?
Seeing that GPU computing finally got traction and that our decision to invest in this technology in 2009, fully commit to this route in 2012, and stick with it in 2015 was right. It was the only correct one, but I'm a bit disappointed that there are currently no viable alternatives on the market for extreme-scale computing.

How could this be changed or improved?
This is a difficult question. Developing new architectures requires large investments over many years. The HPC community has to do a better job in showing what the returns are and why it is worth it. But first, the community has to show that they can adopt new architectures. The GPU resolution shows that this is possible, but it took a long time.

Did you observe new trends that CSCS hasn't picked up on yet, or did you instead see other HPC players picking up CSCS ideas for the future?
Given our early investments in GPU computing and the leadership position we have developed along with our partners, we have naturally encouraged others to follow the path we have taken; specifically, the ideas related to domain specific languages to overcome architectural challenges in complex applications for weather and climate as well as materials science are being adopted elsewhere.

Like many other HPC centres, we discuss data science and big data, but I fear we have not yet figured out how to properly implement the underlying service-oriented architectures necessary for an infrastructure that can support these new trends.

What is the challenge?
Systems used for data science in the cloud are heavily automated. We have shown that this is possible for HPC systems too, but requires a very different setup. Training our staff to cope with these new ways of maintaining systems will be a high priority.

How important are European collaborations for CSCS?
Very important! There is no Swiss science, it is a global endeavour that relies on international collaborations. PRACE, the Partnership for Advanced Computing in Europe, is very important for giving visibility to the high-end of our User Lab program and helps us improve its scientific quality.

Europe is “next door” for most Swiss scientists, and it is quite natural that most collaborations will develop on this continent. Therefore, we need strong European partners; this is in our long-term interest, and we have to support our neighbours. We have to see that new initiatives, such as EuroHPC, respect our contributions to the HPC landscape and stay on target from a technical point of view. Some of the recent trends that are purely motivated by politics worry me. We also have benefited a lot from partnerships with labs in the USA and Japan.

What do you wish for in 2019 for CSCS and your team?
For our users, another successful year in science; for CSCS, I wish for us to have the courage to seize the opportunities we see, even if they appear challenging or disruptive; and at a political level, that the issues with Swiss participation in European projects get sorted out quickly without disrespecting our democratic process.

Prof. Thomas Schulthess
Director of CSCS

Content

KEY INFORMATION

Founded in 1991, CSCS develops and provides the key supercomputing capabilities required to solve challenging problems in science and/or society. The centre enables world-class research with a scientific user lab that is available to domestic and international researchers through a transparent, peer-reviewed allocation process. CSCS's resources are open to academia, and are available as well to users from industry and the business sector.

Production Machines

Piz Daint, Cray XC50, 27.2 PFlops
Piz Daint, Cray XC40, 2.2 PFlops

Granted Resources for User Lab

2018: 46 709 533 node h
2017: 43 451 090 node h

User Community

2018: 132 Projects, 1 584 Users
2017: 116 Projects, 1 213 Users

Employees

2018: 99
2017: 92

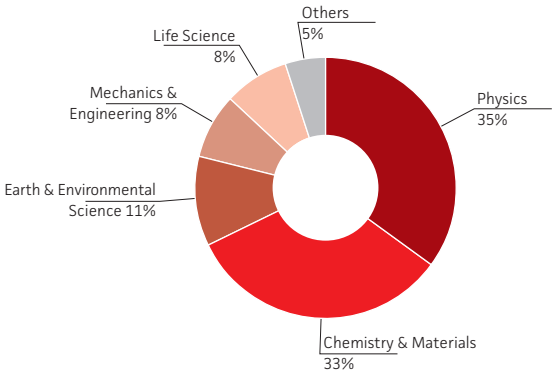
Investments

2018: 2.5 Mio CHF
2017: 4.2 Mio CHF

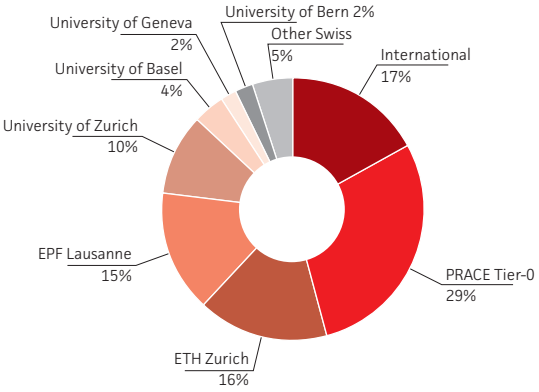
Operational Costs

2018: 19.9 Mio CHF
2017: 16.4 Mio CHF

User Lab Usage by Research Field



User Lab Usage by Institution



Computing Systems Overview

Name	Model	Installation/Upgrades	Owner	TFlops
Piz Daint	Cray XC50/Cray XC40	2012 / 13 / 16 / 17 / 18	User Lab, UZH, NCCR Marvel	27 154 + 2 193
Phoenix	x86 Cluster	2007 / 12 / 14 / 15 / 16	CHIPP (LHC Grid)	86
Piz Kesch	Cray CS-Storm	2015	MeteoSwiss	196
Piz Escha	Cray CS-Storm	2015	MeteoSwiss	196
Monte Leone	HP Cluster	2015	User Lab	7 + 15
Grand Tavé	Cray X40	2017	Research & Development	437

Nora Abi Akar – Software Engineer, Scientific Software & Libraries

Nationality	Lebanese
Working at CSCS since	February 2018
Background	2011-2015 Bachelor in Electrical and Computer Engineering, American University of Beirut, Lebanon 2015-2017 Master's degree in Computer Science, MS Research Scholarship, EPFL
Specialised in	As a software engineer in the Scientific Software and Libraries team at CSCS, I have had the chance to participate in two of our ongoing projects. My main focus has been on the Arbor project. I have worked on optimising the code on the multicore backend by taking full advantage of vectorisation as well as developing a multi-threaded tasking system. I have also explored optimising the GPU code by using CUDA streams. I have always enjoyed working on performance optimisation, and to be able to do that in the context of a big project has been extremely rewarding. My work on the Arbor project extends beyond optimisation, as I take part in maintaining the code as well as adding new features to the library. In addition to Arbor, I have been involved in the Gridtools project. My work with the Gridtools team centers around evaluating new technologies and their performance. This often requires a deep understanding of the architecture, an exercise I enjoy immensely.
Working at CSCS means to me	Having the chance to build optimised software that can take full advantage of the computational resources and, as a result, be able to play a part in advancing scientific research.
What I like most about my work	I am continuously learning and building my skills in a nurturing environment full of brilliant people. Also, having access to one of the largest supercomputers in the world!
What challenges me at my work	Striving to understand the application domain and systems in order to propose the best solution to any task.

Stephanie Frequente – Human Resources Manager

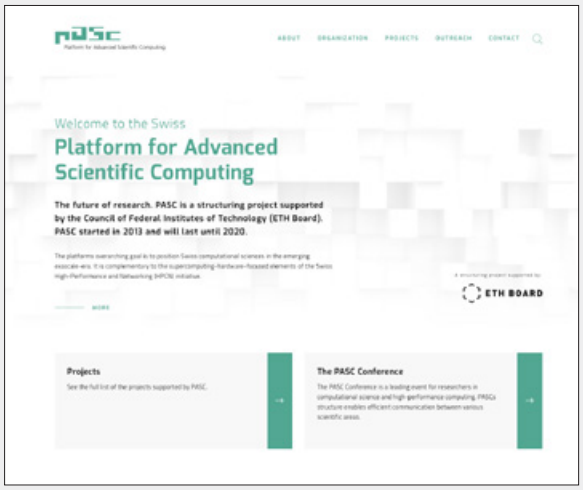
Nationality	Swiss
Working at CSCS since	November 2011
Background	1999-2002 Degree in Hospitality Management, Schweizerische Hotelfachschule Luzern 2007-2008 HR Specialist, Federal Diploma of Higher Education
Specialised in	As Human Resources Manager, I am specialised in recruiting and also developing our employees and managers.
Working at CSCS means to me	It means to support CSCS' strategy and growth from an HR point of view, and to support managers and employee's growth as well as professional development while at the same time making sure that all internal process are adhered to.
What I like most about my work	I love everything about my work at CSCS, and it is very difficult to pick favourite parts. One of my favourite responsibilities is supporting managers in the recruiting process, which means getting to meet candidates from all over the world as well as developing and growing our employees. It is great to work in an international environment and to be able to communicate in three different languages (English, Italian, German) on a daily basis. On top, I particularly cherish the multi-cultural and the academic environment with highly qualified and talented colleagues, as well as the fact that every day I learn something new and that I believe I can really make a difference! Also, at CSCS I have the freedom to bring in new ideas, implement them and continuously drive growth/change. Being embedded in the larger ETH HR team in Zurich is also extremely stimulating, as I am part of interesting projects in cross-functional teams. This drives us forward as an HR team and gives me the opportunity to bring in my experience and ideas as well as learn from my colleagues, and at the same time collaborate and get to know different HR team members.
What challenges me at my work	From my point of view, I am not confronted with challenges, but with opportunities for improvement. For example, bringing together different cultures from different countries with different backgrounds: Internationalisation, globalisation, and last but not least, the impact of digitalisation in our work environment are topics of interest for me.

January

18

New website pasc-ch.org

The website dedicated to the Platform for Advanced Scientific Computing (pasc-ch.org) was redesigned and relaunched. It is now possible to get a quick overview of the activities that have been supported by the initiative.



22

Webinar on best practices for building software on "Piz Daint"

A webinar was organized to help scientists compile their code on "Piz Daint", with a special focus on the EasyBuild template.

25

MAESTRO project accepted in the scope of Horizon 2020

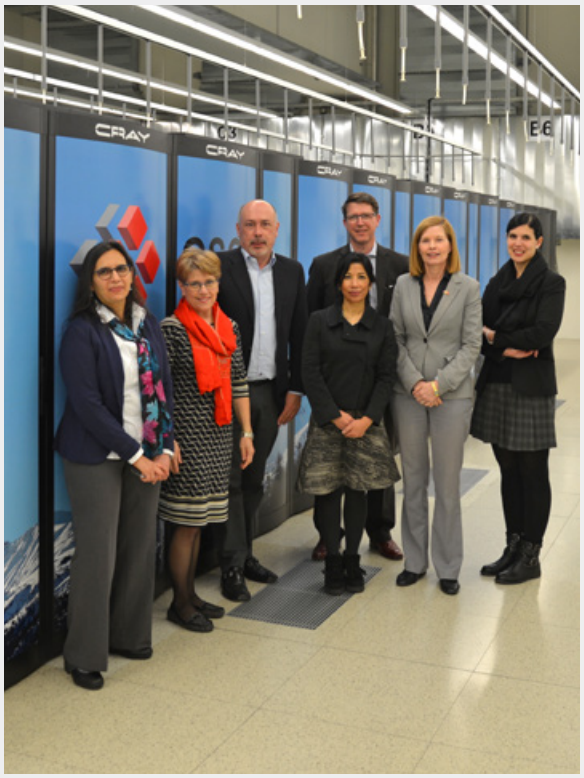
With the participation of CSCS, a European project was accepted in the scope of Horizon 2020 for the duration of three years. The Middleware for memory and data-awareness in workflows (MAESTRO) project will address the ubiquitous problems of data movement in data-intensive applications and workflows.

March

21

Ambassador of Canada to Switzerland and Liechtenstein at CSCS

Mrs Susan Bincoletto, Canada's Ambassador to Switzerland and Liechtenstein in Bern, visited CSCS with a small Canadian delegation and members of the Camera Commercio Ticino.



21 / 23

Workshop on in-situ analysis, visualization with SENSEI and advanced visualization techniques

CSCS organized a two-day course on "in-situ analysis and visualization with SENSEI software", followed by a one-day workshop on "advanced visualization techniques". Attendees learned the basics of in-situ analysis and visualization while being exposed to advanced analysis such as time-dependent autocorrelation and interactive monitoring and steering.

April

09/12

HPC Advisory Council 2018 & HPCXXL User Group

More than 100 professionals attended the ninth Switzerland Conference of the HPC Advisory Council in Lugano. Co-sponsored by CSCS, the conference delved into a wide range of interests, disciplines and topics in HPC – from present day application to future potential. The conference was jointly organized with the HPCXXL User Group (the user group for large HPC installations), a self-organized and sustained group for sites with large scale installations of IBM and/or Lenovo platforms.

10

Euler inauguration

Rui Brandau, Director of IT Services of ETH Zurich, and Carlo Giorgi, Managing Director of HPE Switzerland, inaugurated Euler IV. Housed at CSCS, Euler IV is the central high-performance cluster of ETH Zurich. It was purchased at the end of 2017 and has been in operation since the beginning of 2018.

May

14/15

Workshop on directives-based GPU programming

A two-day course with lectures and exercises introduced the OpenACC programming paradigms for the GPU.

June

13/15

Workshop on exploiting supercomputers and containers for data science

CSCS organized a three-day course focused on data science applications and containerization. Attendees learned how to create and run their own container images and how to make use of containers that are provided by third parties.

20/21

ADAC workshop Switzerland

The sixth Accelerated Data Analytics and Computing (ADAC) workshop organized by CSCS was hosted at the ETH Zurich main building. Leaders in hybrid accelerated HPC in the United States, Japan and Switzerland met to discuss the latest updates in HPC.

24/27

CSCS at ISC18

CSCS and the Swiss HPC community were present this year at ISC18 in Frankfurt. Attendees discovered the latest news about CSCS and HPC in Switzerland while enjoying a cup of coffee and some world-famous Swiss chocolate.

July

02/04

PASC18 in Basel

More than 400 scientists from across the globe met at the fifth edition of the PASC Conference co-sponsored by CSCS and ACM SIGHPC. The topic of the conference was “Fast and Big Data, Fast and Big Computation” and included more than 200 talks.

13

New offices in Via Zurigo, Lugano

A new office has been rented in Lugano to host the increasing number of staff members. The new office space includes 17 work spaces, a meeting room and a small kitchenette.

16/27

CSCS-USI Summer School

This year the CSCS-USI Summer School took place for the first time at the Steger Center for International Scholarship in Riva San Vitale. Among the 21 participants, from Switzerland and abroad, there were undergraduate students, Ph.D. students, postdocs and researchers who attended lectures about High-Performance & Parallel GPU Computing.

September

03

CSCS joins ESiWACE2 project

CSCS received EU funding for a period of four years to contribute to the second phase of the ESiWACE (Centre of Excellence in Simulation of Weather and Climate in Europe) project. The path towards exascale computing holds enormous challenges for the advancement of weather and climate modelling. Issues regarding portability, scalability and data management can hardly be faced by individual institutes. Therefore, ESiWACE2 will link, organise and enhance Europe’s excellence in weather and climate modelling to address these challenges. Within this project, ETH Zurich (CSCS) and MeteoSwiss will collaborate with partner institutions throughout Europe to prepare atmospheric and oceanographic models for the coming generation of computers.

11

User Lab Day 2018

On September 11 in Lucerne, CSCS welcomed more than 70 scientists from Swiss universities and research institutions. Plenary and parallel sessions informed them about current activities and new services provided by the centre. It was also a good opportunity for networking!

October

01/05

EuroHack18: GPU programming hackathon

CSCS organized the fourth GPU-programming hackathon at the Hotel De La Paix in Lugano. The goal of the hackathon is to help and support the researchers in GPU’s programming.

03

Visit of the EU Telecom & Digital Attachés

On October 3, CSCS had the pleasure of welcoming the EU Telecom and Digital Attachés. After the welcome by director Thomas Schulthess, the participants were given a presentation of the CSCS centre including a visit to the machine room and technical infrastructure. This allowed the participants to discover the facilities used in the scope of different EU research projects.

09

Cabinets of "Piz Daint" damaged

"Piz Daint" suffered a serious malfunction as a small fire developed on the wiring and power supply side of a hybrid cabinet. The fire was rapidly extinguished, but it left one hybrid cabinet with major damage and five additional hybrid cabinets with minor internal damage due to the smoke and soot. The affected cabinets were immediately removed and "Piz Daint" went back in production with a reduced configuration until an almost full functionality could be restored a few weeks later.

09/11

Workshop on high-performance computing with Python

A three-day course with lectures and hands-on sessions was offered to show how the programming language Python can be used on parallel computer architectures and how to optimize critical parts of the kernel using various tools.

November

12/15

CSCS at Supercomputing Conference 2018 in Dallas

CSCS and the Swiss HPC community (hpc-ch) had a booth at the world's largest supercomputing conference, SC18, in Dallas, Texas, where they presented the latest HPC developments in Switzerland.

December

01

MaX Centre of Excellence gets additional funding

Since its creation in 2015, CSCS has participated in the Materials at eXascale (MaX) Centre of Excellence. MaX is one of the nine "European Centres of Excellence for HPC applications", funded by the EC under the H2020 e-INFRA-2015 call. MaX supports developers and end users of advanced applications for materials simulations, design and discovery, working at the frontiers of current and future HPC technologies. The EC confirmed additional funding for three years.

Miguel Gila – System Engineer, HPC Operations

Nationality	Spanish
Working at CSCS since	April 2011
Background	1998-2003 Bachelor in Computing Science, University of Almeria, Spain 2006-2008 Master's Degree in Computer Science, University of Almeria, Spain
Specialised in	As a system engineer in the HPC Operations Unit, I'm specialised in administering large computing facilities.
Working at CSCS means to me	Except for maintenance days... it generally means a lot of fun! As a computer geek, I find it amazing having the opportunity to do really interesting things with state-of-the-art technologies, at a scale difficult to find anywhere else. Also, the work environment and culture facilitate balancing work and family life, which, to me, makes CSCS a great place to work.
What I like most about my work	There are many things I love about my job at CSCS, but certainly one of the things that I enjoy the most is resolving complex problems on our systems. Trying to understand why a specific piece of software or hardware is not working as expected, digging all the way through the different layers until finding the root cause, and then reaching a solution, is a fantastic feeling!
What challenges me at my work	Keeping up with technology advancements while making sure our resources are usable and delivered in the most efficient and fair way is an extremely challenging task. It requires constant effort and adaptation to changing situations, which ultimately makes it also very rewarding when things work for our users.

Katarzyna Pawlikowska – Research Collaboration Coordinator, Staff Unit

Nationality	Polish
Working at CSCS since	November 2011
Background	1998-2003 Master's Degree in Economics, Specialisation: International Relations, International Trade, Cracow University of Economics, Cracow, Poland
Specialised in	EU Projects Management, European Collaboration and European policies.
Working at CSCS means to me	To me, working at CSCS means supporting European collaborations that can make an important contribution to a sustainable development of science and our society.
What I like most about my work	CSCS, with its cutting-edge high-performance computing systems, is part of ETH Zurich, one of the top universities in science and technology. This position opens the door to countless opportunities for international collaborations in leading research and innovations. Working here allows me to gain great knowledge in European policies related to the field of digital single market and particularly HPC.
What challenges me at my work	The multicultural environment of CSCS and ETH Zurich together with the diversity of European partners is always very stimulating. Furthermore, being exposed to fields that extend beyond my background and experience is extremely fascinating and continues to drive my thirst for exploration!

User Lab Day 2018 – "Meet the Swiss National Supercomputing Center"

After a few years in which new developments and offers at CSCS were communicated during PASC conferences, we returned to the format of full-day meetings with users, offering plenary and parallel sessions. CSCS welcomed more than 70 scientists on the User Lab Day 2018 in Lucerne.

CSCS wishes to present current activities and new services, to share the mid-term strategy, and to meet with current and prospective future users, creating the opportunity to openly talk about expectations, wishes, and interests. A single session at a PASC conference seems to give not enough time to meet these goals, while a full day offering presentations, personal exchange, and a whole range of mini tutorials on timely topics offers many more opportunities and becomes more attractive for a wider audience.

Vanessa Wood, professor at the Department of Information Technology and Electrical Engineering at ETH Zurich, delivered a keynote lecture on "Adventures of an Experimentalist in the World of Large-Scale Simulations Big Data". During her presentation, Vanessa described how as an experimentalist she started to get interested in simulation and how computers have helped her understand a number of phenomena in the field of colloidal nanocrystals and batteries that experiment alone could not explain.

In another plenary session, CSCS summarized resources and services on offer, updated on the application portfolio, specifying popular codes maintained and upgraded regularly, and offered a glimpse on hardware and other infrastructure behind the scenes, necessary for a large-scale supercomputer like Piz Daint to function as expected.

The rest of the day was dedicated to parallel sessions on a whole range of topics including Debugging & Performance, Compiling, Scientific Visualization, Input/Output Libraries, Workflows and Best Practices (Slurm, Data Transfer, Pre- & Post-processing), Containers, Continuous Integration, Regression Testing, and Interactive Computing. Lunch and coffee breaks as well as a final apéro offered plenty of opportunities for open discussions with the participants.

Resources allocated in 2018

Analysis of usage statistics shows that Chemistry & Materials lost its title of being number one user of resources to Physics for the first time in many years. Physics used 35% of the total allocation, relegating Chemistry & Materials (33%) to second place. Earth & Environmental Science used 11% of the share, Life Sciences and Mechanics & Engineering together 16%, essentially unchanged compared to 2017.

ETH Zurich used 19% of the resources, partially via User Lab Calls and partially via PRACE Tier-0 calls. EPF Lausanne follows at 15%, unchanged from 2017. International utilization went up to 43%, for the most part the PRACE Tier-0 program. Universities of Zurich, Basel, Bern, and Geneva used 10, 4, 2, and 2%, respectively. The remaining 5% of the resources were distributed among other Swiss institutions.

List of CHRONOS Projects Renewals

Principal Investigator	Organisation	Research Field	Project Title	Node h
Constantia Alexandrou	University of Cyprus & Institute of Cyprus	Physics	Nucleon structure using lattice QCD simulations with physical values of the light, strange and charm quark masses	2 000 000
Petros Koumoutsakos	ETH Zurich	Mechanics & Engineering	Simulation of microfluidics for mechanical cell separation: Building the in-silico lab-on-a-chip	2 000 000

List of PRACE Tier-0 Projects

Principal Investigator	Organisation	Research Field	Project Title	Node h
Olaf Kaczmarek	University of Bielefeld	Physics	The chiral limit in (2+1)-flavor QCD	2 342 940
Romain Teyssier	University of Zurich	Physics	Simulating the Euclid Universe	2 000 000
Carmen Domene	University of Bath	Life Science	MICNA – Mechanisms of ion conduction in sodium channels	1 500 000
Gabriel Wlazlowski	University of Warsaw	Physics	Interdisciplinary simulations of Fermi superfluids far from equilibrium	1 281 648
Christoph Schaer	ETH Zurich	Earth & Environ. Science	Convection-resolving climate on GPUs (gpuCLIMATE)	1 185 708
Simone Meloni	University of Rome "La Sapienza"	Chemistry & Materials	ADRENALINE – hAliDe peRovskites sEqueNtiAL deposItioN mEchanism (by ab-initio rare events simulations)	1 147 060
Pierre Ocvirk	University of Strasbourg	Physics	Shining a light through the dark ages	1 000 000
Stefano Vanni	University of Fribourg	Life Science	LDbud – Lipid Droplet Biogenesis	1 000 000
Aaron Walsh	University of Bath	Chemistry & Materials	Overcoming bottlenecks in disordered kesterite photovoltaics (KESTPV)	368 000
Francesco Gervasio	University College London	Life Science	CryptoPocketSim – Understanding the mechanism of cryptic pocket formation at protein-protein interfaces	294 120

Largest Projects (> 500 000 Node h)

Principal Investigator	Organisation	Research Field	Project Title	Node h
Stefan Goedecker	University of Basel	Chemistry & Materials	Structure prediction of solids, surfaces and clusters	1 000 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	Ab-initio exploration of novel 2D materials for logic switch applications and beyond	913 000
Nicola Spaldin	ETH Zurich	Chemistry & Materials	Coupled and competing instabilities in complex oxides	900 000
Lucio Mayer	University of Zurich	Physics	Multi-scale evolution of massive black hole binaries on the fast track with GPUs; from cosmological galaxy mergers to the in-spiral driven by gravitational waves combining SPH and direct N-Body codes	884 672
Nicola Marzari	EPF Lausanne	Chemistry & Materials	Mapping the structures and properties of all bulk forming binary systems: A high-throughput study	804 000
Ulrike Lohmann	ETH Zurich	Earth & Environ. Science	The impact of aerosols in the past, present, and future climate	746 608
Marcella Iannuzzi	University of Zurich	Chemistry & Materials	Ab-initio nanofluidics: Electronic structure and transport	720 000
Sandra Luber	University of Zurich	Chemistry & Materials	Advancing biomimetic water oxidation catalysis via novel Co(II)-based cubanes	700 000
Carlo A. Pignedoli	Empa	Chemistry & Materials	Screening of the electronic and optical properties of carbon based 1D heterostructures	690 000
Antoine Georges	University of Geneva	Chemistry & Materials	Electronic and structural properties of complex oxides: Vanadates, iridates and cuprates	665 600
Nicola Marzari	EPF Lausanne	Chemistry & Materials	Materials for energy	600 000
Sandra Luber	University of Zurich	Chemistry & Materials	Advancing electronic structure calculations for complex nature-inspired systems	599 000
Jürg Hutter	University of Zurich	Chemistry & Materials	Properties of liquids, solutions, and interfaces from density functional theory	590 000
Andrew Jackson	ETH Zurich	Earth & Environ. Science	Self-excited dynamo action in planets	500 720
Andreas Fichtner	ETH Zurich	Earth & Environ. Science	Multiscale global Earth model II	500 000
Dimitri Komatitsch	CNRS Marseille	Mechanics & Engineering	The «CLEAR IMAGE» Project, going beyond the current state-of-the-art in seismic imaging	500 000

Angelo Mangili – Account Manager, User Engagement & Support

Nationality	Swiss
Working at CSCS since	December 1991
Background	1983-1988 Bachelor in Computer Science, EPFL 1989-1991 Research assistant, Computer Graphics Laboratory, EPFL
Specialised in	Currently my role at CSCS is account manager in the User Engagement and Support Unit. My background is 3D data visualization and software development. As one would imagine, I started at CSCS supporting users in visualising simulation results and in pre- and post-processing of data. Then my career evolved to general application support and currently into account management. My technical expertise allows me to be the liaison between CSCS and selected external customers, such that both needs and expectations are properly understood and represented. It is now a number of years that I have been the account manager for MeteoSwiss, a challenging customer for whom CSCS provides a broad range of services, which go far beyond simple computational resources. For this reason, part of my work consists of finding adequate solutions that meet all of a customer's needs and requirements. Mutual understanding and trust are important aspects of the work and are essential in customer relationships, and they are gradually developed over time.
Working at CSCS means to me	Being able to help advance and promote science for the benefit of the entire society, and also being given a unique opportunity to be part of the catalyst process, which enables technology development and innovation.
What I like most about my work	Each customer has its own needs and expectations, which often vary and increase over time. Moreover, technology is rapidly changing, thus the proposed solutions will never last for more than a couple of years. We are in the position of having to regularly reassess these needs and requirements and proactively propose better alternatives. This is what makes working at CSCS exciting!
What challenges me at my work	When new customers approach us, very often it is a challenge to fully understand the extent of their needs and expectations. We have to clearly explain what CSCS is actually able to offer, and we ultimately rise up to the challenge of thinking of possible solutions or new services that were never addressed nor offered before. Sometimes we try to push customers' limits, even if it might cause some disruption in their workflow, but the achievements are often highly rewarding both for the customer and for us.

Maxime Martinasso – Computer Scientist, Office of the CTO

Nationality	French
Working at CSCS since	July 2014
Background	1998-2001 Bachelor in Computer Science, University of Avignon, France 2001-2003 Master in Computer Science Fundamentals and Graph Theory, University of Bordeaux 1, France 2004-2007 Ph.D. in HPC and Communication Modelling, INRIA, France
Specialised in	In the office of the CTO, our main goal is to technically lead the centre towards the strategic goals provided by the director. As a computer scientist and CTO deputy in the office of CTO, I am responsible for assisting the CTO in identifying, planning and executing technical decisions to learn and apply new technologies, and also to oversee the development of key initiatives inside the centre to implement these strategic goals. My role varies from writing proposals for Swiss and European projects, to developing proofs-of-concept for certain technologies, to leading teams to apply or implement successful tools and techniques, and to disseminating the resulting solutions in international conferences or work groups.
Working at CSCS means to me	CSCS is a well-recognized and a very innovative centre in the HPC community. It was one of the first to introduce GPGPU at large scale specifically for operational weather forecasting systems, and it became a leader in that field. Today, one of CSCS's goals is to converge Cloud and HPC technologies together, which brings very exciting and technical challenges. CSCS also provides a very stable and nice working environment. Both aspects make CSCS a great place to develop and deploy future technology to improve the HPC community.
What I like most about my work	Being part of CSCS in the office of the CTO is a very interesting position, as on one hand I need to have a deep understanding of the HPC technology and its community, and, on the other hand, I need to identify innovative ways to meet CSCS's technical objectives. I like the fact that I have a great flexibility in terms of work directions with a wide variety of technical topics to investigate. I also appreciate the fact that I can rely on very knowledgeable and professional colleagues.
What challenges me at my work	There are different aspects which challenge me, and, most importantly, I like very much the diversity of these challenges. For instance, I may need to focus on a complex technical problem for a couple of weeks or do networking and dissemination activities by participating in international conferences. I also need to be aware of technological developments and their potential applications, and I evaluate the benefits of vendor-provided technology.

List of Projects by Institution

Chalmers University of Technology

Continuum models for Brownian motion in weakly rarefied flows, using the Immersed Boundary Method (IBM) on GPU, Andreas Mark (Mechanics & Engineering, 33 000 node h)

CNRSf Marseille

The «CLEAR IMAGE» Project, going beyond the current state-of-the-art in seismic imaging, Dimitri Komatitsch (Mechanics & Engineering, 500 000 node h)

Cornell University

Phase-stability of superconducting intermetallics from quantum Monte Carlo simulations, Maximilian Amsler (Chemistry & Materials, 400 000 node h)

Empa

Effects of membranes composed of phosphatidylcholine, phosphatidylserine and cholesterol, on calcium phosphate ion association and aggregation: An in-silico and in-vitro investigation, Riccardo Innocenti Malini (Chemistry & Materials, 95 892 node h)

Forward and inverse modelling of greenhouse gases, Dominik Brunner (Earth & Environmental Science, 129 000 node h)

EPF Lausanne

Computational design of novel immunogens for vaccine development, Bruno Correia (Life Science, 451 320 node h)

GPU-SPHEROS: GPU accelerated meshless solver for Pelton turbine sediment erosion, Ebrahim Jahanbakhsh (Mechanics & Engineering, 300 000 node h)

The evolution of rough surfaces in the adhesive wear regime, Jean-François Molinari (Earth & Environmental Science, 300 000 node h)

Advanced fast ion auxiliary heating scenarios in two- and three-dimensional tokamak and stellarator magnetic topologies, Jonathan Graves (Physics, 225 000 node h)

Machine learning of dielectric response tensors, David Wilkins (Chemistry & Materials, 224 000 node h)

Mechanical properties of hybrid halide perovskite photovoltaics: Monitoring humidity-induced degradation with computer simulations, Wanda Andreoni (Chemistry & Materials, 800 000 node h)

Role of conformational dynamics in protein-protein interactions, Matteo Dal Peraro (Life Science, 90 000 node h)

2D Materials for gas separation, Varoon Kumar Agrawal (Chemistry & Materials, 165 600 node h)

Grid-based gyrokinetic simulations for studying basic turbulent transport mechanisms and realistic confinement properties of tokamak plasmas, Stephan Brunner (Physics, 450 000 node h)

Machine learning of chemical shifts, Edgar Engel (Chemistry & Materials, 308 100 node h)

Exploring excited state properties of metal organic frameworks for sensing and photocatalysis, Berend Smit (Chemistry & Materials, 200 000 node h)

Novel topological phases of materials, Oleg Yazyev (Chemistry & Materials, 175 632 node h)

Mapping the structures and properties of all bulk forming binary systems: A high-throughput study, Nicola Marzari (Chemistry & Materials, 804 000 node h)

Materials for energy, Nicola Marzari (Chemistry & Materials, 600 000 node h)

Simulations of drifting and blowing snow over East Antarctica using the Weather Research and Forecasting (WRF) model, Michael Lehning (Earth & Environmental Science, 112 000 node h)

Simulation of plasma turbulence in the periphery of tokamak devices, Paolo Ricci (Physics, 425 000 node h)

Atomic scale processes at solid-water interfaces, Alfredo Pasquarello (Chemistry & Materials, 430 000 node h)

Construction of a reference database for a neural network potential to model permeation of CO_2 in a metal organic framework, Rocio Semino (Chemistry & Materials, 50 000 node h)

ETH Zurich

Improvement of performance of axial turbines through geometric optimization using high fidelity CFD, Reza Abhari (Mechanics & Engineering, 62 240 node h)

Three-dimensional imaging of the crust-mantle interactions beneath the Hangai Mountains, Mongolia using magnetotellurics, Alexey Kuvshinov (Earth & Environmental Science, 145 000 node h)

3D seismic wave simulations for the Mars InSight mission, Martin van Driel (Earth & Environmental Science, 200 000 node h)

Carrier dynamics in nanocrystals and nanocrystal solids, Vanessa Wood (Chemistry & Materials, 165 852 node h)

Uncertainty quantification for three-dimensional compressible fluid flows, Siddhartha Mishra (Computer Science, 346 000 node h)

Multiscale global Earth model II, Andreas Fichtner (Earth & Environmental Science, 500 000 node h)

Tunneling contributions to the proton switching mechanism of porphycene on metallic surfaces with ab-initio ring polymer instantons, Jeremy Richardson (Chemistry & Materials, 246 000 node h)

High-resolution glacier modelling with PISM, Julien Seguinot (Earth & Environmental Science, 90 000 node h)

Pulling it off – deciphering the vinculin F-actin catch bond, Viola Vogel (Life Science, 257 000 node h)

Multiphase fluid flow, evaporation and crystallization in deforming porous materials, Jan Carmeliet (Mechanics & Engineering, 185 000 node h)

Land-climate feedbacks in a changing climate, Edouard Davin (Earth & Environmental Science, 228 000 node h)

Multiscale in-silico modelling of bone mechanoregulation: From molecule to cell, tissue and organ, Harry van Lenthe (Life Science, 40 000 node h)

Self-excited dynamo action in planets, Andrew Jackson (Earth & Environmental Science, 550 720 node h)

Ab-initio exploration of novel 2D materials for logic switch applications and beyond, Mathieu Luisier (Chemistry & Materials, 913 000 node h)

Coupled and competing instabilities in complex oxides, Nicola Spaldin (Chemistry & Materials, 900 000 node h)

Imperial College London

A priori evaluation of grid resolution for turbulent boundary layer using Flux-Reconstruction schemes, Yoshiaki Abe (Mechanics & Engineering, 384 000 node h)

Leiden University

The origin of the compact, dusty objects G1 and G2 at the galactic center, Simon Portegies Zwart (Physics, 80 000 node h)

Michigan State University

Gravitational wave and neutrino signals from core-collapse supernovae and failed supernovae, Kuo-Chuan Pan (Physics, 200 000 node h)

Paul Scherrer Institute

Precise simulations of multi bunches in high-intensity cyclotrons, Andreas Adelmann (Physics, 123 000 node h)

Reaction pathways modelling of conversion of methane over zeolite catalysts, Dennis Palagin (Chemistry & Materials, 155 000 node h)

High-fidelity characterization of safety parameters of Generation-IV European Sodium Fast Reactor optimized core using Serpent 2 Monte Carlo code, Alexander Ponomarev (Physics, 50 000 node h)

Computational investigation of radiation damage in thorium oxide-based fuel matrices, Raoul Aurelien Ngayam-Happy (Chemistry & Materials, 36 000 node h)

SUPSI

Computational design and Optimization of Dendron-sirna complexes for the treatment of rheumatoid Arthritis (CODA), Marco A. Deriu (Life Science, 35 532 node h)

Università della Svizzera italiana

Kinetics of urea decomposition in aqueous solution via enhanced ab-initio molecular dynamics, Daniela Polino (Chemistry & Materials, 270 000 node h)

Computational design of tailored peptidomimetics targeting the mRNAs translation process: The next-generation of therapeutic anticancer molecules, Daniele Di Marino (Life Science, 90 000 node h)

Atrial fibrillation in-silico study, Simone Pezzuto (Life Science, 200 000 node h)

University College Cork

Photoactive metal organic frameworks, from understanding to design, Davide Tiana (Chemistry & Materials, 34 200 node h)

University of Basel

Adaptive ensemble calculations for reaction barrier energies and transition states for quantum machine learning and alchemical perturbations in chemical space, Guido F. von Rudorff (Chemistry & Materials, 100 000 node h)

Effects of complex liquid environments on material properties, Giuseppe Fisicaro (Chemistry & Materials, 400 000 node h)

University of Bern

Flavour singlet physics from lattice QCD in fully physical conditions, Urs Wenger (Physics, 430 000 node h)

Modelling extreme events in multiple ocean ecosystem stressors (M-OceanX), Thomas Frölicher (Earth & Environmental Science, 100 000 node h)

Pleistocene climate variability – complex modeling of the earth system, Christoph Raible (Earth & Environmental Science, 300 000 node h)

University of California at Berkeley

A novel distributed-memory framework for neural network training, Kurt Keutzer (Computer Science, 300 000 node h)

University of Fribourg

Large-scale molecular modeling of lipid droplet biology, Stefano Vanni (Life Science, 300 000 node h)

University of Geneva

Magnetism in novel 2D materials, Marco Gibertini (Chemistry & Materials, 300 000 node h)

Instrument Monte Carlo Simulations for the Dark Matter Particle Explorer (DAMPE), Andrii Tykhonov (Physics, 32 000 node h)

Electronic and structural properties of complex oxides: Vanadates, iridates and cuprates, Antoine Georges (Chemisty & Materials, 665 600 node h)

University of Lausanne

3D numerical thermo-mechanical modelling of tectonic nappe formation with application to the Helvetic nappe system, Stefan Markus Schmalholz (Earth & Environmental Science, 50 000 node h)

Identification of protonation events that drive activation and desensitization of acid-sensing ion channels, Stephan Kellenberger (Life Science, 36 000 node h)

University of Melbourne

Compressible Direct Numerical Simulations on Impinging Jet Flows, José Otero (Mechanics & Engineering, 80 000 node h)

High-fidelity simulation of high-pressure turbine for model development using machine learning, Richard Sandberg (Mechanics & Engineering, 300 000 node h)

University of Parma

Ab-initio estimation of contact hyperfine fields in muon spin rotation spectroscopy: Towards a new DFT assisted method for long range magnetic structure determination, Roberto De Renzi (Chemistry & Materials, 22 480 node h)

University of Rome "La Sapienza"

Boiling of nanostructured surfaces: Effect of wetting and roughness, Mauro Chinappi (Mechanics & Engineering, 80 000 node h)

Ionic and electroosmotic flow in conical nanopores, Mauro Chinappi (Chemistry & Materials, 100 000 node h)

University of Twente

Sheared Rayleigh-Bénard convection – towards the ultimate regime of turbulence, Detlef Lohse (Mechanics & Engineering, 99 441 node h)

University of Zurich

Computing renal oxygenation in realistic vascular networks for improved treatment of anemia associated with chronic kidney disease, Kartik Jain (Mechanics & Engineering, 36 000 node h)

Ab-initio nanofluidics: Electronic structure and transport, Marcella Iannuzzi (Chemistry & Materials, 720 000 node h)

Multi-scale evolution of massive black hole binaries on the fast track with GPUs; from cosmological galaxy mergers to the in-spiral driven by gravitational waves combining SPH and direct N-Body codes, Lucio Mayer (Physics, 884 672 node h)

Molecular Dynamics simulations of a-Synuclein binding to physiological membranes, Davide Mercadante (Life Science, 50 000 node h)

Solving large-scale overlapping generation models with stochastic fiscal policy, Simon Scheidegger (Others, 132 000 node h)

Predictive models for galaxy formation, Romain Teyssier (Physics, 200 000 node h)

Advancing understanding and design of photosensitizers for artificial water-splitting, Sandra Luber (Chemistry & Materials, 98 000 node h)

ZHAW

Generation of synthetic turbulence and stochastic backscatter to improve the quality of Hybrid RANS-LES turbulence models, Marcello Righi (Mechanics & Engineering, 36 000 node h)

Renewals

Empa

Screening of the electronic and optical properties of carbon based 1D heterostructures, Carlo A. Pignedoli (Chemistry & Materials, 690 000 node h)

EPF Lausanne

Multiscale Simulations of Biological Systems and Bioinspired Devices, Ursula Röthlisberger (Life Science, 418 472 node h)

Halide perovskites for solar cells: In-silico design of novel materials, Ursula Röthlisberger (Chemistry & Materials, 331 456 node h)

ORB5 – Core and pedestal turbulence, Laurent Villard (Physics, 370 000 node h)

Cardiac and vascular numerical simulations, Simone Deparis (Computer Science, 350 000 node h)

ETH Zurich

Simulation of microfluidics for mechanical cell separation: Building the in-silico Lab-on-a-Chip, Petros Koumoutsakos (Mechanics & Engineering, 2 000 000 node h)

Learning and optimization for collective swimming, Petros Koumoutsakos (Mechanics & Engineering, 360 000 node h)

Bayesian uncertainty quantification for large-scale predictive simulations in nanotechnology and life sciences, Petros Koumoutsakos (Computer Science, 150 000 node h)

Cloud cavitation collapse in turbulent flows, Petros Koumoutsakos (Mechanics & Engineering, 320 000 node h)

The impact of aerosols in the past, present, and future climate, Ulrike Lohmann (Earth & Environmental, 746 608 node h)

Investigation of prechamber-induced ignition of natural gas using direct numerical simulations, Christos E. Frouzakis (Mechanics & Engineering, 300 000 node h)

Ab-initio simulations of conductive bridging memristors for application as plasmonic optical switches, Mathieu Luisier (Chemistry & Materials, 386 000 node h)

Aerosol cloud interactions and cloud variability on the regional scale, Jan Henneberger (Earth & Environmental Science, 224 332 node h)

Simulations of stable water isotopes in the atmospheric water cycle with COSMOiso in tropical, midlatitude and polar regions (TROMIPOiso), Franziska Aemisegger (Earth & Environmental Science, 61 200 node h)

General large batch methods for scalable and accurate neural network training, Torsten Hoefler (Computer Science, 120 000 node h)

Paul Scherrer Institute

Dissolution, growth and ion uptake at phyllosilicate surfaces: Coupling atomistic interactions at the mineral-water interface with Kinetic Monte Carlo model, Sergey Churakov (Earth & Environmental Science, 320 000 node h)

Università della Svizzera italiana

Homo- and heterodimerization mechanism of chemokines receptors CCR5 and CXCR4 investigated by Coarse-Grained Metadynamics simulations, Vittorio Limongelli (Life Science, 240 000 node h)

University of Basel

Doped insulators at high-pressure as the new high-temperature superconductors, José A. Livas-Flores (Chemistry & Materials, 350 400 node h)

Structure prediction of solids, surfaces and clusters, Stefan Goedecker (Chemistry & Materials, 1 000 000 node h)

Atomization energies from ab-initio calculations without empirical corrections, Dirk Bakowies (Chemistry & Materials, 240 000 node h)

University of Bern

ISOCARBON (Modelling ISOtopes of CARBON in the Earth System), Fortunat Joos (Earth & Environmental Science, 99 360 node h)

Structure, elastic constants and thermal expansion of iron at Earth's core conditions from free energy calculations, Donat Adams (Earth & Environmental Science, 80 000 node h)

University of Cyprus & Cyprus Institute

Nucleon structure using lattice QCD simulations with physical values of the light, strange and charm quark masses, Constantia Alexandrou (Physics, 2 000 000 node h)

University of Geneva

Relativistic cosmological simulations with gevolution, Martin Kunz (Physics, 300 000 node h)

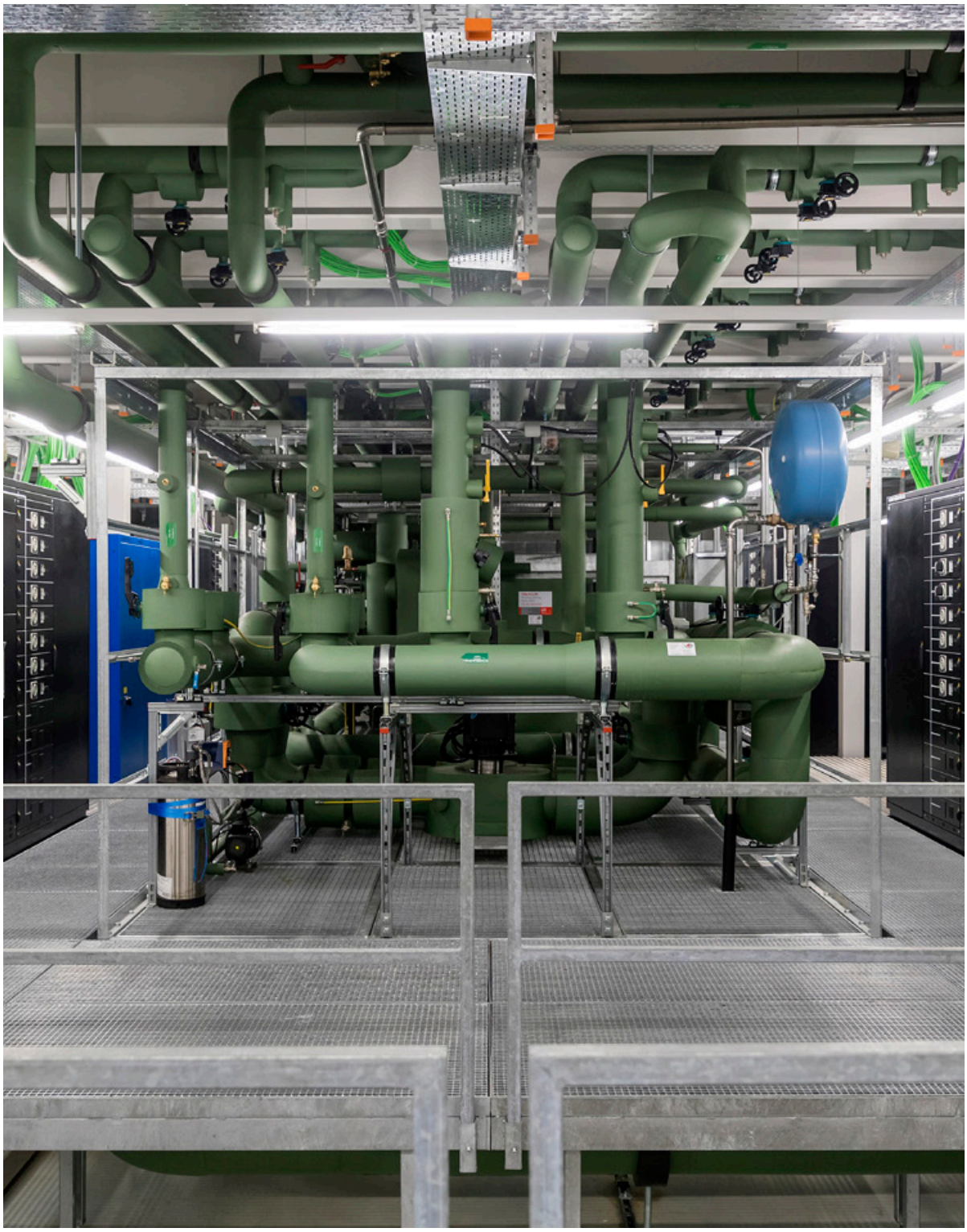
University of Zurich

CP2k program development, Jürg Hutter (Chemistry & Materials, 96 000 node h)

Properties of liquids, solutions, and interfaces from density functional theory, Jürg Hutter (Chemistry & Materials, 590 000 node h)

Advancing biomimetic water oxidation catalysis via novel Co(II)-based cubanes, Sandra Luber (Chemistry & Materials, 700 000 node h)

Advancing electronic structure calculations for complex nature-inspired systems, Sandra Luber (Chemistry & Materials, 599 000 node h)



Economists cash in on efficient high-performance computing method

Macroeconomic models, designed to study for example monetary and fiscal policy on a global scale, are extremely complex with a large and intricate formal structure. Therefore, economists are using more and more high-performance computing to try and tackle these models.
(Image: William Potter, Shutterstock.com)

Macroeconomic models, designed to study for example monetary and fiscal policy on a global scale, are extremely complex with a large and intricate formal structure. Models can quickly reach hundreds of dimensions. The two main sticking points in calculating such complex economic models are recursively approximating the high-dimensional functions using many iteration steps and at the same time, systems of non-linear equations must be solved at millions of grid points that describe the model.

To find a highly efficient solution method that can recursively calculate the economic decision-making rules (known as policy functions), researcher from University of Zurich and Università della Svizzera italiana combined so-called sparse grids with a high-dimensional model reduction framework. The resulting linear combination of sparse grids, which describe the model and thus the policy functions, are nested together like a Russian doll, and are lined-up in such a way that they optimally approximate and describe the original high-dimensional space.

The code to calculate the individual grids and their combination is highly parallelised. Even in small models with "only" 50 dimensions, the method efficiently scales up on "Piz Daint" to as many as 1 000 computer nodes at the same time. To further minimise the time required to solve the functions and keep communication between the processors and the processes running on them highly efficient, the researchers also used a hybrid parallelisation scheme (Message Passing Interface and Intel® Threading Building Blocks.).

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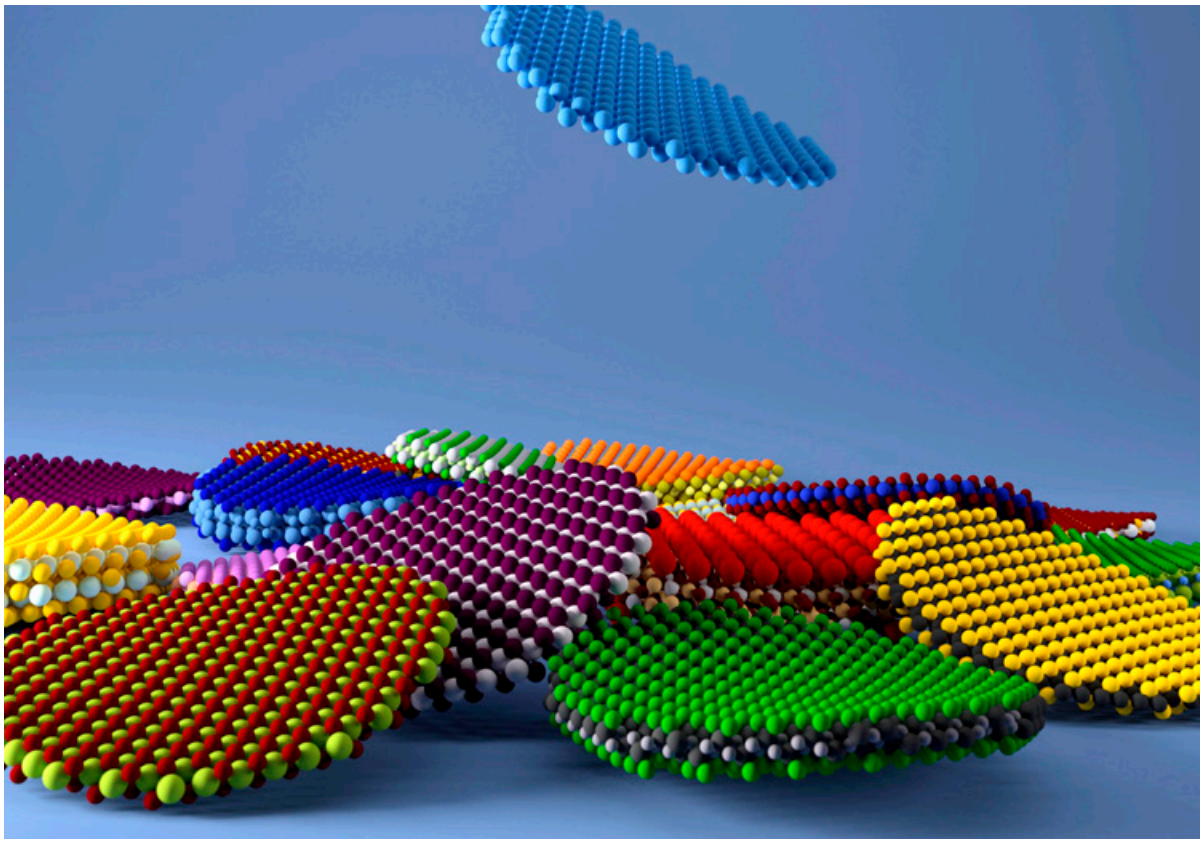
Fishing with simulations for two-dimensional materials



Computational discovery of novel 2D materials. (Image: Giovanni Pizzi, EPFL)

Researchers from EPF Lausanne have developed a method that used "Piz Daint" supercomputer to identify 258 promising candidates for two-dimensional compounds in one go. Two-dimensional materials are ascribed completely different physical properties to the three-dimensional compounds from which they derive. They are thus promising candidates for the next generation of electronic and optoelectronic applications.

The scientists began their investigation with 108 423 materials known from other experiments. They first used their self-developed algorithm to filter out materials with suitable geometric properties: crystals with a layered structure. This helped them to narrow down the number to 5 619 compounds, which were then screened using high-throughput electronic structure calculations, thus fishing out materials whose layers only had weak bonding interaction between them.

Using this step-by-step approach and further testing the crystals' mechanical stability, vibrational properties, electronic structure and potential magnetic strength the researchers succeeded in identifying the 258 promising candidates.

Ever since the successful production of graphene, two-dimensional materials have been intensively researched. But until now, only a few dozen could be produced or exfoliated from three-dimensional materials. The success of the new method in the search for two-dimensional materials is a perfect example of how computational methods can speed up the discovery of new materials.

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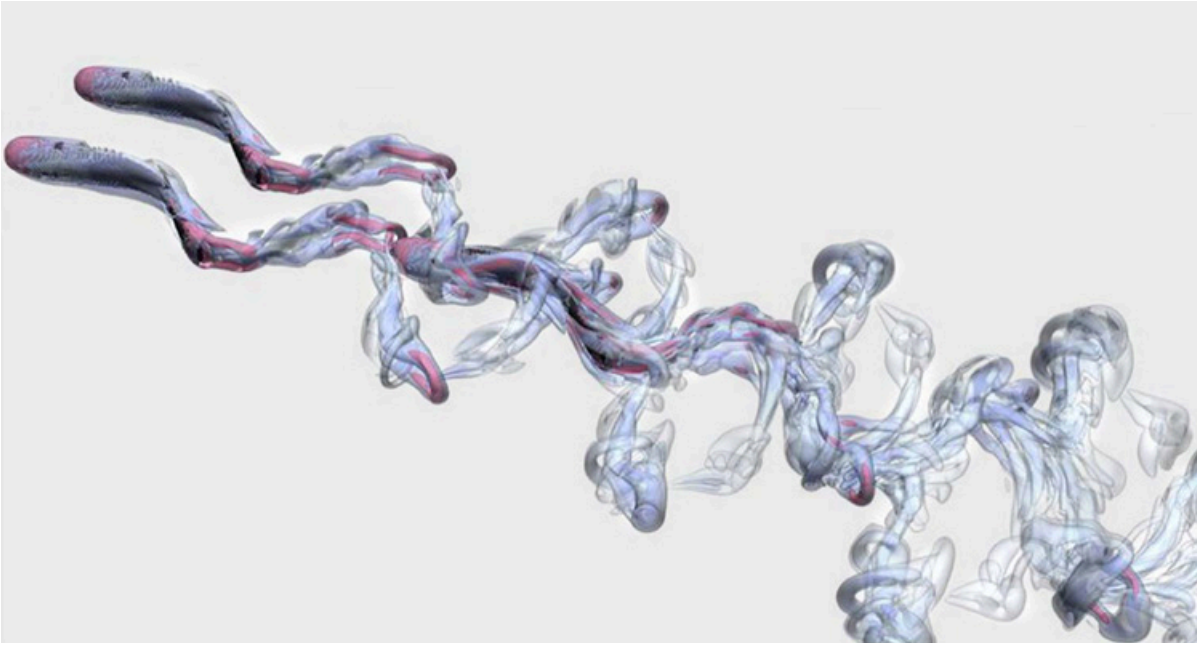
Swimming in schools saves energy



A follower interacts judiciously with the wake generated by two leading fish, which increases its swimming-efficiency substantially. (Image: CSElab/ETH Zurich)

Researchers from ETH Zurich's Computational Science & Engineering Lab (CSElab) combined on "Piz Daint" supercomputer for the first time high-accuracy flow simulations of the complex interplay between swimming fish and their flow environment with reinforcement learning, a potent machine learning algorithm. This kind of learning algorithm has been used in games such as 'Go', enabling the computer to outperform humans. Deploying reinforcement learning on complex physical systems, however, has never been done before, as the algorithm requires thousands of iterations.

Fish schooling was previously only tackled with very simplified models that did not account accurately for the fluid dynamics of the fish swimming. With these simulations they answered the longstanding question of whether fish gain an energetic advantage by swimming in schooling formations – and the answer is "yes."

The researchers determined that the fish swam most energetically when they swam not one after the other, as previously suggested, but at an offset from the swimming direction of the leader.

At such locations they harnessed the vortices generated by the leader by intercepting them with their head, splitting the vortex into fragments that they then guided down their bodies. The progress of these fragmented vortices supplies the fish with thrust without robbing the leader of energy.

The developed algorithms and physics learned can be transferred into autonomously swimming or flying robots. Autonomous robot swimmer or flyer could handle unexpected flow situations – for example, when flying between buildings in high winds to deliver goods, or during search and rescue operations in stormy conditions. The possibility of letting airplanes with similar destinations fly in formation along certain routes to save fuel is also being considered. The algorithms developed in this work could also be put to use here.

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Simulations for InSight Mars mission

Artist's rendering of the InSight lander. The sensor assembly of the seismometer (underneath the protective shield) is pictured at the front left. (Image: NASA/JPL-CALTECH)

Why have Earth and Mars developed so differently although their original structure and chemical composition seem so similar? How large, thick and dense are the core, mantle and crust? What is their structure? On 26 November 2018, the NASA "InSight"-lander - equipped with a special seismometer - landed on Mars in order to answer these questions.

Researchers from ETH Zurich and the Swiss Seismological Service, who were involved in developing the seismometer's electronics, are now among the first to analyse and interpret the data recorded by the seismometer. As seismic waves on Mars have never been recorded with such a sensitive seismometer, numerical simulations were the only way to prepare for the data evaluation of the NASA InSight mission. On the "Piz Daint" supercomputer they calculated seismic wave propagation for around 30 different Mars models.

Depending on the planet's internal structure, the waves travel at different speeds and take different routes from the source to the seismometer. The time it takes for the waves to travel through Mars' interior will help the scientists to better understand the planet's structure and rock properties.

The visualisation of one of the numeric simulations shows how the waves travel along the surface of Mars, orbiting around the planet and passing the lander three times. It is essential to measure the waves on each of the three passes, as this will allow the scientists to gather information about the planet, identify the timing and location of the Mars quake, and to calculate its approximate structure, all with just one seismic station.

The calculated models are used to check how certain structures, such as the crustal thickness, influence the measurements. The models thus help the researchers to verify their methods and to better understand seismograms on Mars. In order to finally understand the Martian structure, the ETH researchers will compare the actual measurements with the simulated data. For this, they will draw on the Mars model catalogue to see if and how the measurement changes, taking into account the models, what the structures are and what all the simulations have in common.

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Vasileios Karakasis – Scientific Computing Support Group Lead, User Engagement & Support

Nationality	Greek
Working at CSCS since	September 2015
Background	2000-2005 Diploma in Electrical and Computer Engineering, National Technical University of Athens, Greece 2005-2006 Research Assistant, Computing System Laboratory, National Technical University of Athens, Greece 2007-2012 Ph.D. in High-Performance Computing, National Technical University of Athens, Greece
Specialised in	Since November 2018, I have been leading the Scientific Computing Support Group after I worked for three years as an HPC Application Specialist in the same group. As group lead, I manage the activities of my team to enable our user community to make the best use of the HPC environment that CSCS is providing. My specialization is performance engineering and regression testing. I have been mentoring teams in GPU Hackathons organized by the center and acted as the lead developer of a framework for regression testing and continuous integration of HPC applications. I have been furthermore involved in directive-based GPU programming, representing the center in the OpenACC technical committee. I have been supporting and helping our users in using OpenACC and I have taught GPU programming in seminars held by our center, as well as in a summer school co-organized with USI.
Working at CSCS means to me	Enabling science, by helping our users and providing them the resources for running efficiently on one of the biggest supercomputer systems in the world.
What I like most about my work	What I do like the most about my job is that there is not a regular routine. I enjoy working with my team in supporting our users so they can run their codes optimally on our system, testing and benchmarking codes, designing and implementing solutions for our users' workflows, as well as designing and developing our software tools.
What challenges me at my work	My team at CSCS is essentially a production engineering team with knowledge that spans the whole software stack, from systems and computer architecture to scientific applications. Anything we do has a direct impact on the users of the center, so everything counts. Given the complexity and the scale of such a large center, this is a big challenge.

Rolando Summermatter – Facility Manager, Business Services

Nationality	Swiss
Working at CSCS since	October 2011
Background	1990-1994 Electrician apprenticeship 2001-2003 Specialised Diploma in Building installations (HVAC) 2008-2010 Diploma of Electrical Installation Mastery
Specialised in	As a facility manager in the Business Services Unit, I am responsible for ensuring that technical and infrastructural installations are maintained according to the standards, that they are efficient, and that a well-functioning IT infrastructure is always present at CSCS. It is my task to keep the installations up-to-date and propose improvements where needed. This implies continued specific, individualised training depending on the sector of activity, which may vary between electrical engineering and cooling installation. Over the years I have spent at CSCS, I have had the opportunity to expand my knowledge of datacenter infrastructures, which is very different from a conventional technical infrastructure. I have also been able to refine and expand my knowledge in electrical engineering thanks to multiple projects and analyses carried out on the installations.
Working at CSCS means to me	For me, working at CSCS represents a great opportunity and immense luck, as it gives me the opportunity to work with a competent team. I get updated continuously, and I have the opportunity to carry out diversified activities made interesting also by the evolution of the technologies.
What I like most about my work	CSCS offers a pleasant environment in which you never stop learning.
What challenges me at my work	My main challenge is to keep up with the ever-changing technologies and to continue to investigate new topics to ensure that I am stimulated.

“If users are happy, we are happy, and we can consider ourselves successful”

After her Postdoc in Chemistry at ETH Zurich, Maria Grazia Giuffreda started working at CSCS in 2006 as a support specialist in the group responsible for user support. In 2010 she was promoted to Group Leader of the User Support team, and then she became Associate Director and head of the User Engagement and Support Unit in 2013. As a group leader, she has now served the user community for about 9 years. In this interview, Maria Grazia Giuffreda gives insight into her challenging work, into the work of her team and, last but not least, into user development during the last decade.

Maria Grazia Giuffreda, Associate Director and head of the User Engagement and Support Unit, during the interview done by Simone Ulmer, editor Science & Technology at CSCS.

Maria Grazia, are you bored after nearly a decade of user support?
Maria Grazia Giuffreda: It is difficult to be bored in this role (laughs). CSCS has always been a very dynamic workplace. With enthusiasm and readiness to get involved and be challenged, there is really no space for boredom. I cannot remember a single quiet year since I have taken over User Support. Every couple of years there is a new flagship system being installed or upgraded, at other times there is a new user community coming in, a new software stack, new services. Frequent changes are common in High-Performance Computing and data centers that are at the forefront of innovation and technology, like CSCS.

What does a Head of User Engagement and Support at CSCS do? What does your normal day look like?
I am responsible for the User Lab Program, including proposal submissions, and I am the liaison with the User Lab scientific community. Furthermore, I have account managers reporting to me on paying customers, and I am responsible for PRACE Tier-0 proposal calls. On a typical day I receive several emails from PIs and users asking me questions that need my attention, and I am involved in multiple meetings with colleagues and other leadership team members.

I coordinate the activities of two groups, Scientific Computing Support and Compute and Data Services Support, with weekly discussions with the group leaders. I am also responsible for the account management team who is taking care of the relationships between CSCS and the paying customers, making sure that needs and expectations from both parties are met. Additionally, I supervise help desk activities, problem intervention, and user communication.

You mentioned PRACE, the Partnership for Advanced Scientific Computing in Europe, where CSCS is a hosting member of a so-called Tier-0 system. What does this mean?
The objective of PRACE is to enable high-impact scientific discovery and engineering research and development across all disciplines, to enhance European competitiveness for the benefit of society, and to provide a persistent pan-European High-Performance Computing service and infrastructure. Being a hosting member in this organization means that CSCS is offering world class computing and data management resources to scientists all over Europe and seeking to promote challenging and ambitious science.

In PRACE, Swiss scientists can receive access to extreme-scale computing resources of different architectures. Together with Switzerland, currently the other hosting members are France, Italy, Germany and Spain.

Are there other European collaborations involving CSCS?
The beauty of working in this field is that science has no borders. Scientists and experts in extreme computing and data science thrive on collaborations and joint ventures. This is why CSCS is involved in a number of European and international collaborations, such as the European Centers of Excellence for HPC applications, MaX (Materials at eXascale), ESiWACE2 (Excellence in Simulation of Weather and Climate in Europe), the Human Brain Project, MAESTRO (Middleware for memory and data-awareness in workflows), and PLAN-E (Platform of National eScience/Data Research Centers in Europe), to name a few.

Users from the User Lab scientific community apply for free resources, but customers are users buying computing time without application?
Academic users can get access to computational and data resources for free, but they have to present high-quality projects that their peers deem to be worth pursuing. In particular, CSCS organizes two national calls for proposals each year and participates in two annual European PRACE Tier-0 calls. Proposals submitted to the national calls are first scrutinized by in-house experts for their technical soundness and feasibility and then sent to two scientific reviewers from academic institutions abroad. Based on these assessments, an independent expert committee ranks the proposals and makes recommendations on allocations of computer time, which the Director of CSCS has so far always followed in making final decisions. The painstaking procedure is designed to guarantee that all projects be treated equally and that all promising projects can be implemented on high-performance computers. Alternatively, users have the choice to buy resources and so become paying customers of CSCS. Allocations are then granted without peer review; however, used funds will typically come from funding organizations that implement their own selection process.

We are talking about 1 500 users. How many people take care of them, or in other words, how large is your team?
There are 20 members in the User Engagement and Support Unit. This might look like a lot but, actually, being part of this team does not mean that all we do is answer tickets from users.

The team does tremendous work to keep the system healthy from a user's point of view. The team recently assembled a professional regression suite, known as Reframe, to check the status of the system, and they have been so successful that other centers are starting to adopt their work flow and other teams within CSCS are starting to use it for their own daily work. The team has automated the installation of applications and scientific libraries such that, whenever there are major upgrades, we can easily reinstall and recompile our supported software stack. The team also prepares procedures for users to help them install their own applications easily. Furthermore, team members are working on benchmark suites for the production system and they are looking into new cloud services that CSCS is starting to provide, including continuous integration and interactive computing. What perhaps is not clear is that being part of the support team comes with a huge responsibility; after all, we take care of the core business of CSCS: If users are happy, we are happy, and we can consider ourselves successful.

"User Engagement" sounds like a challenge.
It depends on what we mean by User Engagement. For me it means to have an open channel with the user community. I am very excited by the User Lab Day, which we re-introduced in 2018. It is important that members of our user community know that there is an opportunity to come and discuss with us their wishes and their requests, and to make sure that they understand that we value their opinion. On the other hand, it is also of absolute importance for CSCS to reach out and present new services being offered. In my opinion, we cannot detach ourselves from our users. We need to make sure that we convey our messages, inform about our strategies, visions, and services, and work together with users who play a vital role in ensuring our success through supporting their outstanding science in the most effective way.

I assume there are users with a lot of experience as well as newcomers. How specific to a particular person is the user support?
The very experienced users are often considered collaborators more than anything else. They come to us with very high-level issues that regularly require the effort of both parts to diagnose and to solve, but we also get in touch with them when we need their help, for example when testing new services in pre-production.

Newcomers are more likely to require our assistance to get started. There are numerous ways in which we support them, for instance with an interactive tool on our user portal that generates job scripts custom-tailored to their needs. We also offer webinars that help them get started at CSCS. Our webpage provides instructions and information on a range of topics. Furthermore, we offer courses that are relevant to new users. I think the bottom line is that all users are important. There are no silly or intelligent questions, there are just questions; and we are there to help our users to get the most out of our resources.

Has your job changed over the years, or has it stayed pretty much the same?
The job has certainly changed as it needs to adapt to the rapid advances in hardware and software technology. Responsibilities and even the strategy of CSCS as an organization may change whenever new services are implemented. I am always behind my team and find it very important to discuss changes in daily work as well as in medium-term goals. This may not be as obvious for other units, but whatever we do has an immediate impact on our user community. Whatever we deploy as tools, any new service has to be robust, well-thought out and well-planned. We do not have the freedom to simply test and see how it goes, because the impact on the users will be immediate and non-negligible. Our services are evolving, and therefore also are the responsibilities that come with it. Even in the user program, I face challenges at times when new scientific disciplines join our user community. Their requirements may be quite different from those that we are used to, and we may need to implement new tools, software, and services and even adapt proposal submissions.

In addition to user support, another challenging part of your work is your involvement in the distribution of computing time. You are a kind of "interface" between user and Scientific Advisory Board. What is the biggest challenge for you in that role?
This is something that I really enjoy doing. I like to look at proposals and find expert scientific reviewers, even though this requires a lot of time and concentration. We have an excellent Scientific Advisory Board who meticulously discuss every proposal based on technical assessment at CSCS and scientific review. The biggest challenge for me is to convey the right messages to the applicants concerning the outcome of their project proposals. There is a lot of competition for HPC resources on Piz Daint, and therefore only the very best projects are granted full allocation.

Lower-ranked proposals need to be cut in allocation and some proposals need to be rejected. Proper response to the latter is not always easy, however, it is important to let applicants know why their proposals were cut or rejected so they rest assured that their proposal was considered seriously and they find ways to improve their chances in future calls.

In addition to the daily business of your group, CSCS offers a wide range of training courses for users. Can you briefly name the most important ones?
Every year we develop a training program that includes new offerings covering new tools and technology, as well as courses we have repeatedly offered over the years due to their proven importantance to many of our users. In 2019 we are offering courses on: Distributed TensorFlow, Scientific Python, GPU programming, OpenACC (in our Summer School), Interactive supercomputing (Jupyter and similar services), Advanced C++, and HPX as well as visualization.

Is the large spectrum of courses a consequence of the increasingly complex technologies and the increasingly complex scientific questions that researchers want to solve with the help of simulations, or are there other reasons?
We are trying to help our users to deploy our production systems in the most effective way, therefore we offer courses in parallel computing on GPUs among others. On the other hand, we also want to make users aware of new technologies and new services that they might not be aware of but may prove useful to them, or that they might know of but not in as much detail as is necessary to tap their full potential.

Has the user behavior changed during your many years of experience?
Of course, users always want to do their research as soon as possible, and, if possible, just "now". Still I have noticed growing awareness of the complexity of running a computer center successfully, of offering stable and reliable HPC and storage resources. Users have definitely shown a growing readiness to collaborate with us and contribute to making our services as useful as possible. I think that these days, more than ever before, they see us as their peers, not on a scientific level, but for issues regarding the technical realization of their scientific projects.

As you mentioned earlier, CSCS re-introduced the user day in 2018. The annual user meeting offered — besides a scientific presentation of ETH-professor Vanessa Wood and insights into the work of CSCS behind the curtain — for the first time workshops on various topics, at which CSCS experts answered questions from the audience. This was very well received.

What was the trigger for the new programme, which offered plenty of room for discussion?
We want to reach out to our users. We wish to make them aware of new services in place at CSCS. In other words, we need to move forward but we want the community to evolve with us and not be left behind to catch up only later. The new format establishes better communication needed for CSCS to know about changing user needs and for users to learn about future plans of CSCS. We also need to reach out to scientists that have not yet used HPC but might well benefit of it. The User Lab Day is the day where everybody can "meet the Swiss National Supercomputing Centre" to openly discuss wishes, visions, and services.

Will next year's programme again have such a broad spectrum of topics or has the success inspired even more new ideas?
We will certainly repeat the format with parallel sessions to cover those topics that are important for CSCS and for our users. We are finalizing the program based also on feedback from the participants and the users.

If you made a wish for the CSCS users, what would it be?
Looking at the future, I wish for a community of users and customers that continues to be open-minded, like only scientists and dreamers can be, that embraces whatever new technologies and evolutions come our way, and that willingly accepts the challenges and the opportunities rather than looking back and wishing for what can no longer be, as nice as it might have been.

Impressions of the the CSCS User Lab Day 2018

On September 11 in Lucerne, CSCS welcomed more than 70 scientists from Swiss universities and research institutions to plenary and parallel sessions designed to inform about current activities and new services provided by the centre.

On the lakeshore of "Vierwaldstättersee" in sunny Lucerne, CSCS staff welcomed scientists from Switzerland and across Europe to the CSCS User Lab Day 2018. More than 70 participants from Swiss universities and research institutions attended plenary and parallel sessions in which the centre informed about current activities and new services. Ample time and opportunity for networking was allotted during coffee and lunch breaks and during an apéro just after the last session.

In her welcome address, Maria Grazia Giuffreda, Head of User Engagement and Support, encouraged attendees to use the opportunity for networking. "On the one hand, CSCS is here to present activities and new services, and to share the mid-term strategy, but on the other hand, we wish to meet all of you face-to-face and talk openly about expectations and wishes".

The official program started with an inspiring lecture delivered by Vanessa Wood, professor at the Department of Information Technology and Electrical Engineering at ETH Zurich: "Adventures of an Experimentalist in the World of Large-Scale Simulations Big Data". Afterward, the plenary presentations of CSCS staff outlined the resources and services offered by CSCS and used by scientists from all major Swiss research institutions.


ETH zürich
Adventures of an Experimentalist in the
World of Large Scale Simulations and Big Data
Professor Vanessa Wood
Department of Information Technology and Electrical Engineering, ETH Zurich
CSCS User Lab Day
September 11, 2018


CSCS

Finances

User Lab Expenditures & Income

	Expenses CHF
Investments	**2 472 847.05**
Equipment and Furniture	**36 602.15**
Personnel	**10 479 422.83**
Payroll	8 082 858.03
Employer's Contributions	1 452 619.20
Further Education, Travel, Recruitment	943 945.60
Other Material Expenses	**8 162 250.28**
Maintenance Building & Technical Infrastructure	431 896.60
Energy	2 383 238.73
Administrative Expenses	7 438.26
Hardware, Software, Services	4 323 130.14
Remunerations, Marketing Workshops, Services	511 615.24
Other	504 931.31
Extraordinary Expenditures	**1 215 548.59**
Membership Fees	58 461.46
PASC Initiative Contribution External Projects	1 157 087.13
Total Expenses	**22 366 670.90**

	Income CHF
Basic Budget Income	**25 347 909.33**
ETH Zurich Operations	18 997 909.33
ETH-Rat - HPCN Investments	5 000 000.00
ETH-Rat - PASC Initiative Software Development	1 350 000.00
Other Income	**151 784.32**
Services / Courses	73 447.24
Reimbursements	18 810.88
Other	59 526.20
Total Income	**25 499 693.65**
Balance	**3 133 022.75**

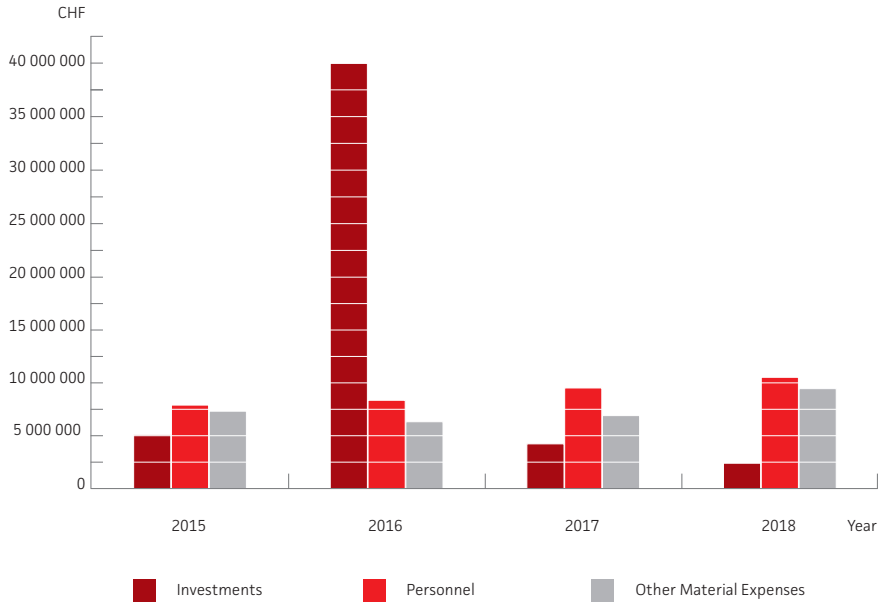
.+. Rollover Project Fund PASC & IAAS 2017	823 415.70
./. Rollover Project Fund PASC & IAAS 2018	820 881.91
Total Balance User Lab 2018 Operational Funds & HPCN Investments - Transferred back to ETH Zurich 31.12.2018	**3 135 556.54**

Third-Party Contributions

	CHF
Third-Party Contributions	**10 953 871.30**
EU Projects (excl. 2/3 overhead ETH Zurich)	4 003 075.00
MeteoSwiss	2 187 000.00
Blue Brain Project	1 119 917.00
CHIPP	1 022 547.00
PRACE High-Level Support Team	773 856.60
IAAS	749 000.00
University of Zurich	304 000.00
Paul Scherrer Institut	277 200.00
MARVEL	205 000.00
Hilti	178 265.00
NCCR MARVEL / SNF	65 711.70
Università della Svizzera italiana	36 000.00
University of Geneva	20 000.00
Partner Re	12 300.00

User Lab Expenses Development (CHF)

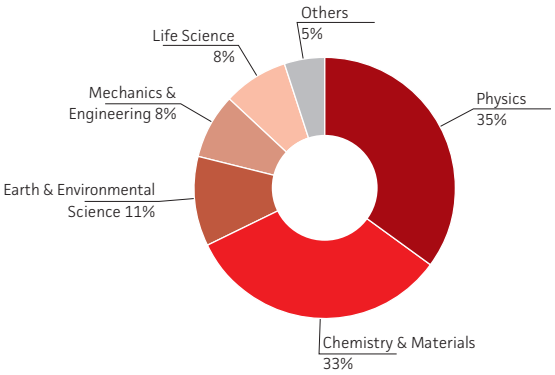
	2015	2016	2017	2018
Investments	5 042 501	40 023 533	4 218 973	2 472 847
Personnel	7 842 930	8 313 178	9 478 260	10 479 422
Other Material Expenses	7 271 103	6 293 094	6 877 461	9 414 401



Usage Statistics

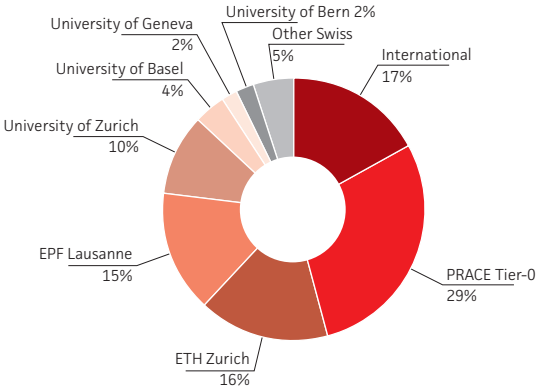
User Lab Usage by Research Field

Research Field	Node h	%
Physics	15 537 867	35
Chemistry & Materials	14 370 198	33
Earth & Environmental Science	4 736 388	11
Mechanics & Engineering	3 650 101	8
Life Science	3 308 827	8
Others	2 175 327	5
Total Usage	**43 778 708**	**100**



User Lab Usage by Institution

Institution	Node h	%
International	7 327 101	17
PRACE Tier-0	12 598 014	29
ETH Zurich	7 201 448	16
EPF Lausanne	6 532 008	15
University of Zurich	4 229 333	10
University of Basel	1 840 126	4
University of Geneva	941 616	2
University of Bern	749 782	2
Other Swiss	2 359 280	5
Total Usage	**43 778 708**	**100**



Compute Infrastructure

Computing Systems Overview

Name	Model	Installation/Upgrades	Owner	TFlops
Piz Daint	Cray XC50/Cray XC40	2012 / 13 / 16 / 17 / 18	User Lab, UZH, NCCR Marvel	27 154 + 2 193
Phoenix	x86 Cluster	2007 / 12 / 14 / 15 / 16	CHIPP (LHC Grid)	86
Piz Kesch	Cray CS-Storm	2015	MeteoSwiss	196
Piz Escha	Cray CS-Storm	2015	MeteoSwiss	196
Monte Leone	HP Cluster	2015	User Lab	7 + 15
Grand Tavé	Cray X40	2017	Research & Development	437

Computing Systems Specifications

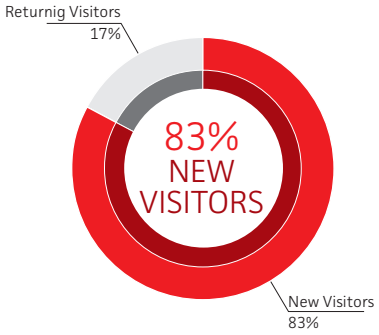
Name	Interconnect Type	CPU Type	No. Cores	No. Sockets per Node	No. Nodes
Piz Daint	Cray Aries	Intel Xeon E5-2690 v3 + Nvidia P100 Intel Xeon E5-2695 v4	12 18	1 + 1 2	5 704 1 813
Phoenix	Infiniband FDR	Intel Xeon E5-2670 Intel Xeon E5-2690 Intel Xeon E5-2680 v2 Intel Xeon E5-2680 v4	8 8 10 14	2 2 2 2	64 1 48 40
Piz Kesch	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2 + 8	12
Piz Escha	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2 + 8	12
Monte Leone	10 Gb Ethernet	Intel Xeon E5-2667 v3 Intel Xeon E5-2667 v3 Intel Xeon E5-2690 v3 + Nvidia K40C	8 8 12	2 2 2 + 1	6 7 4
Grand Tavé	Cray Aries	Intel Xeon Phi CPU 7230	64	1	164

Communications Statistics

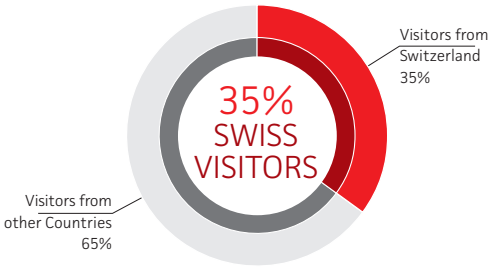
Website cscs.ch

	2017	2018
Total Website Visitors	87 678	76 265
Average Website Visits (Minutes)	2:49	2:22

New Visitors



Visitors Origin



Top 5 Most Visited Website Pages

1. CSCS Homepage www.cscs.ch
2. Open Positions www.cscs.ch/about/open-positions/
3. Staff www.cscs.ch/about/staff
4. Piz Daint www.cscs.ch/computers/piz-daint/
5. Computers Dismissed https://www.cscs.ch/computers/dismissed/

Twitter

	2017	2018
Followers	866	1 097

LinkedIn

	2017	2018
Followers	6 164	6 810

YouTube

	2017	2018
Watch Time (Minutes)	568 872	613 000
Average View Duration (Minutes)	4:41	5:21
Number of Views	121 234	114 600

Facebook

	2017	2018
Followers	139	181

CSCS in the News

	2017	2018
News Websites	334	341
Print	159	196
Radio & TV	12	7

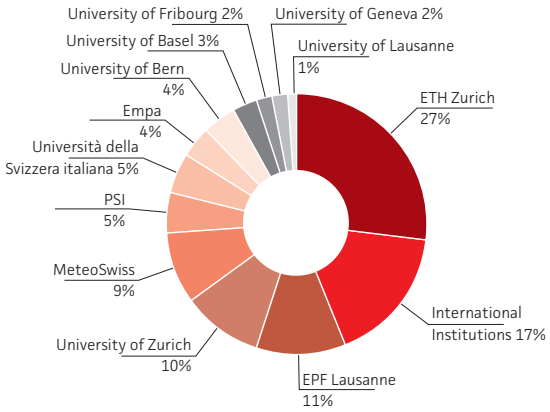
Word Cloud of News Related to CSCS

User Satisfaction

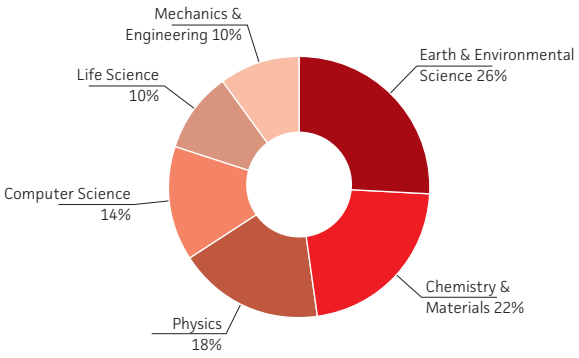
A user satisfaction survey was submitted to 1 584 users in January 2019. The response rate was of 14.9% (236 answers).

User Profile

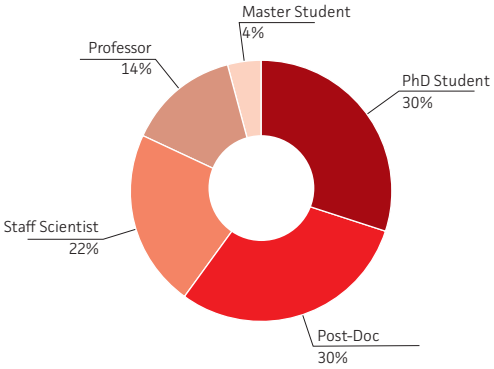
Your institution



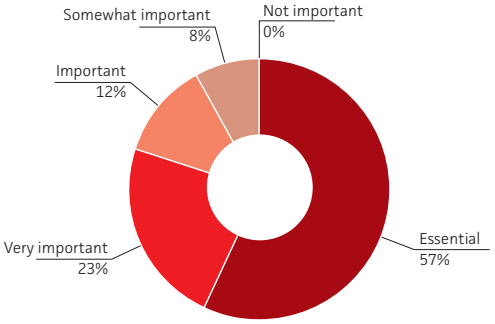
Your scientific field



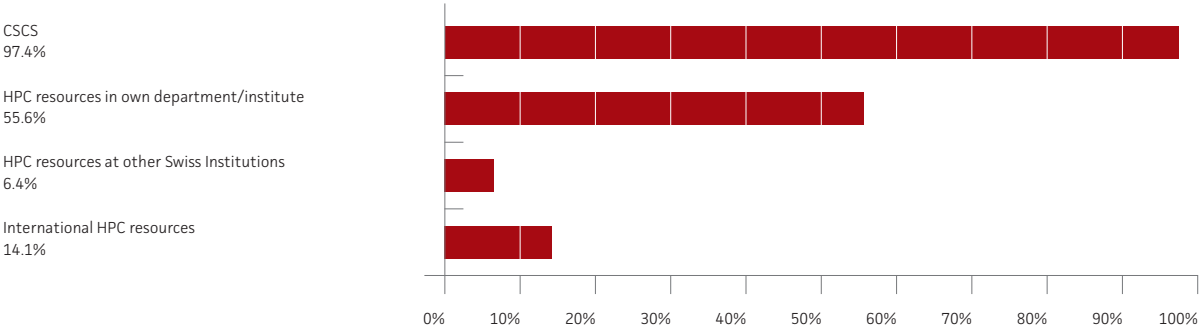
Your position



For my research, CSCS resources are

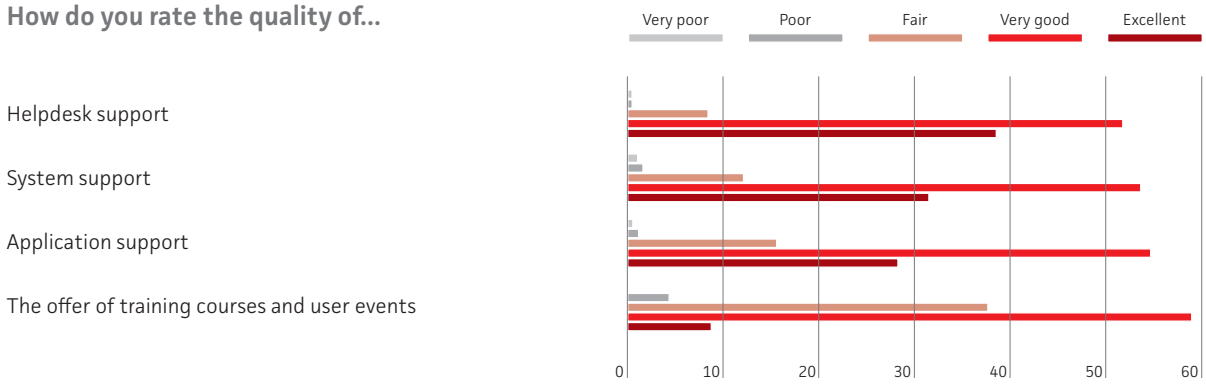


Which HPC resources are you using?

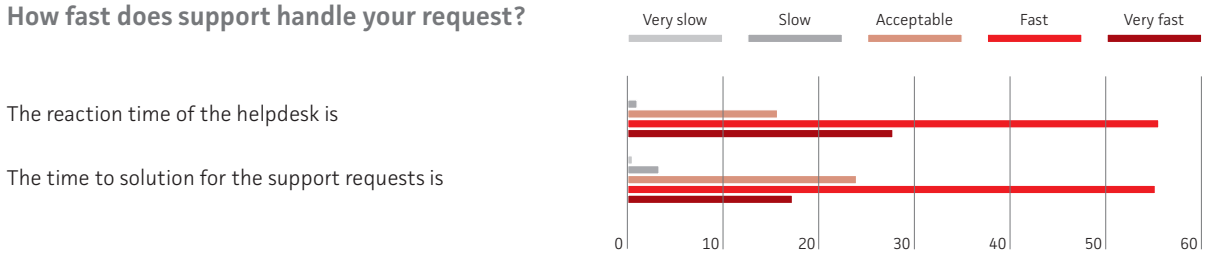


User Support

How do you rate the quality of...

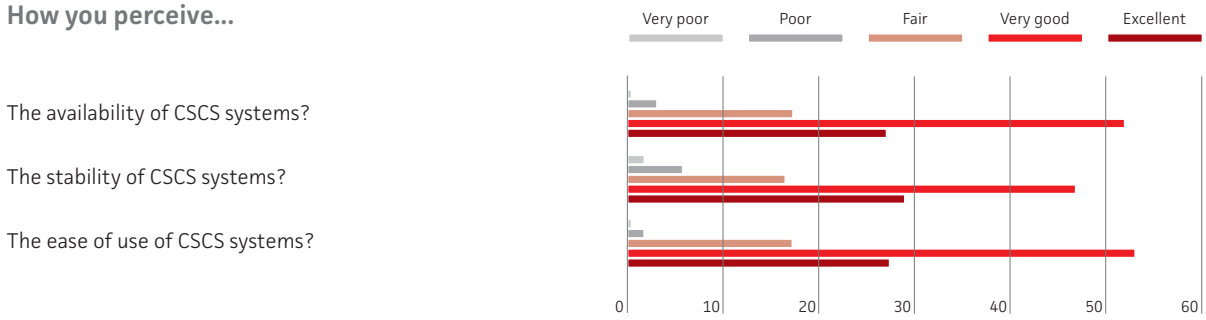


How fast does support handle your request?

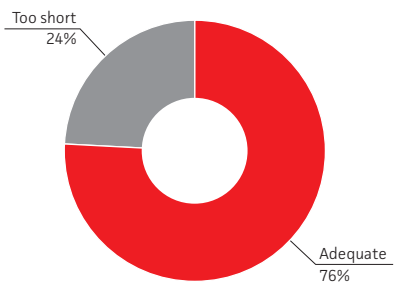


System Availability, Stability and Usability

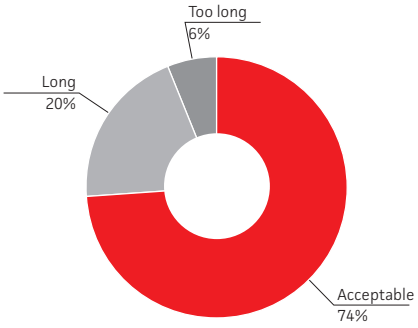
How you perceive...



The run time limits for batch jobs are

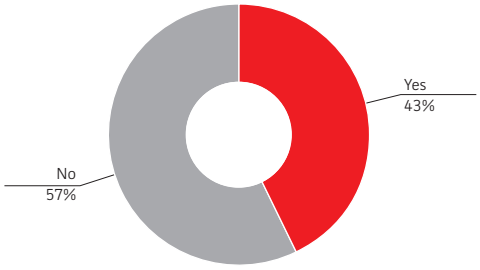


The job waiting time in the queue is

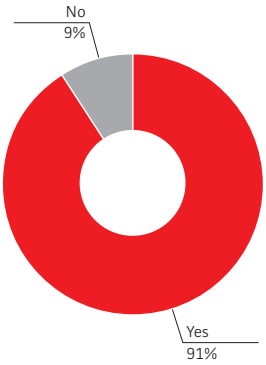


Project Proposal Process

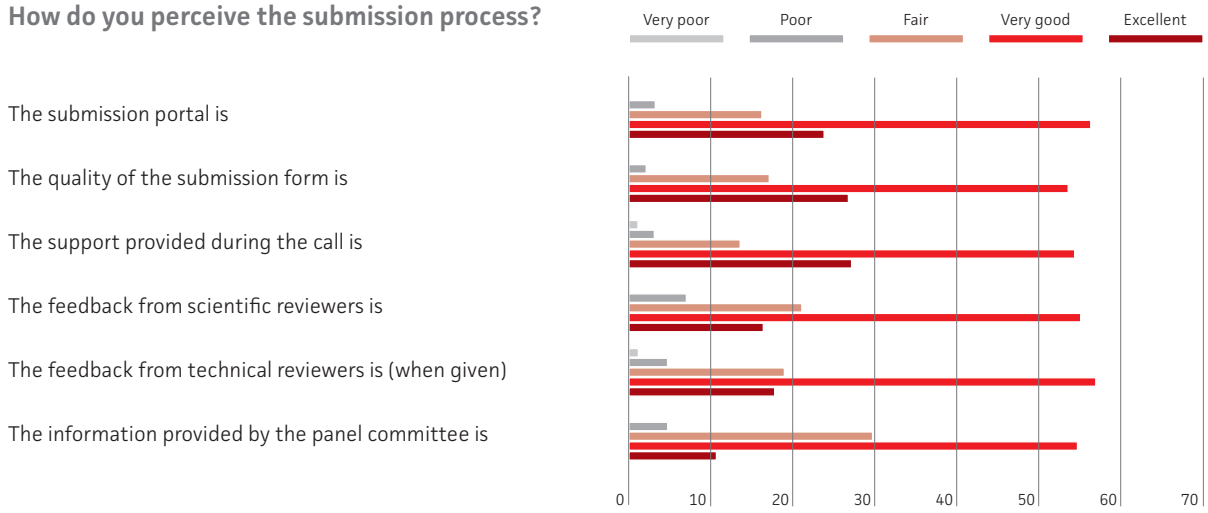
Have you been submitting project proposals to CSCS (as PI or supporting the PI?)



Is the reviewing process transparent?

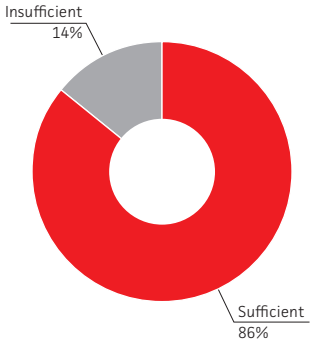


How do you perceive the submission process?

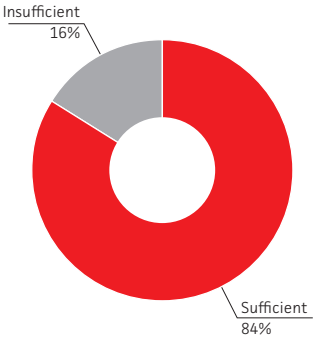


Adequacy of Allocated Resources

The resources assigned to my project are

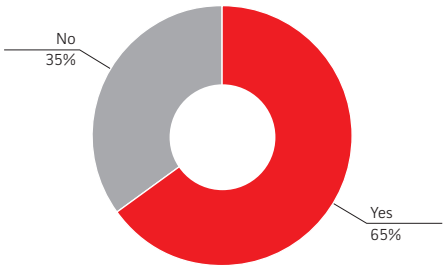


My storage allocation on "project" is

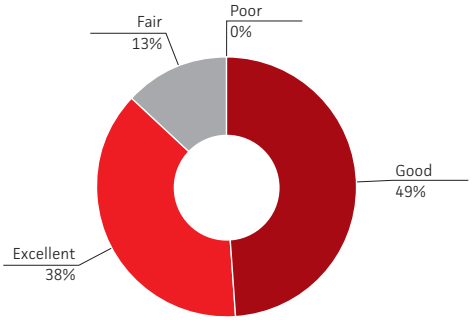


Application Development

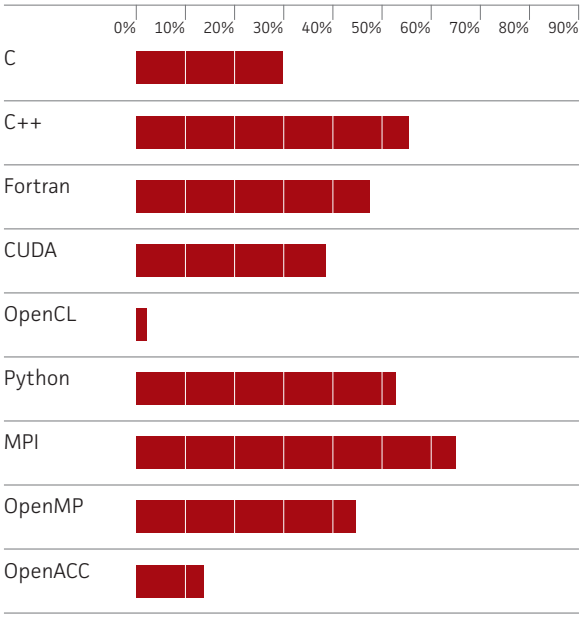
Do you develop and maintain application codes?



How do you rate the offered range of programming tools (compilers, libraries, editors, etc.)?



Which programming languages and parallelization paradigms are you using primarily?



Information & Communication

How do you feel informed about...

Status of the systems

Software and applications

Hardware configuration

Available computing resources

Own allocations

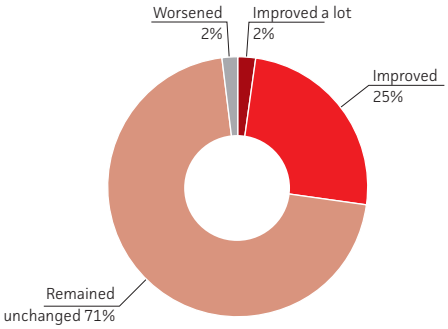
Your consumption of your allocation

Upcoming events and courses

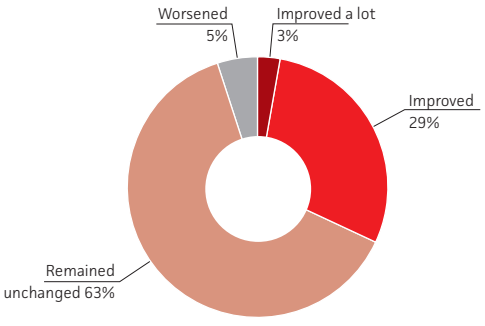
Future developments at CSCS

Perception of CSCS

How has the communication between CSCS and the user community developed during last year?



My general view in the last year is that CSCS (systems, services, support) has

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